Pine Chemicals Association, Inc.

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AR201-13653

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The Honorable Christine Todd Whitman
Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Attention: Chemical Right-to-Know Program

Re: Response to Comments and Amendments to Pine Chemicals Association, Inc. Test Plan for Tall Oil Fatty Acids and Related Substances

Dear Ms. Whitman:

The Pine Chemicals Association, Inc. (PCA) HPV Task Force is pleased to submit its response to comments received on its April 2001 Test Plan for Tall Oil Fatty Acids and Related Substances. We have carefully reviewed the comments submitted by the Environmental Protection Agency (EPA) and the Physicians Committee for Responsible Medicine (PCRM) in November and October 2001, respectively. This document responds to those comments and amends our April 2001 Test Plan. We have organized the submission by subject matter in the same order as our Test Plan.

RESPONSE TO COMMENTS & AMENDMENTS TO TEST PLAN

Categorization of Substances / Selection of Test Material

PCA proposed to group six substances in its Tall Oil Fatty Acids and Related Substances Test Plan. Under this Test Plan, PCA proposed to test tall oil fatty acids (CAS # 61790-12-3) ("TOFA") to represent the category based on its production volume and use of this substance as a raw material for most of the other category members.

EPA suggested that PCA may want to form a separate category comprised solely of monomer acid (CAS # 68955-98-6) and octadecanoic acid (CAS # 68201-37-6). The Agency believes that the test results for TOFA may not be representative of these two members of the category due to the branched and linear nature of the compounds. The Physicians Committee for Responsible Medicine (PCRM)[1], on the other hand, criticized

[1] PCRM's comments were also submitted on behalf of People for the Ethical Treatment of Animals, the Humane Society of the United States, the Doris Day Animal League, and Earth Island Institute.

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PCA for not expanding the category to include seven additional substances from its Test Plan for Tall Oil and Related Substances.

After carefully considering these comments, PCA believes that its categories should remain as originally proposed based upon the explanations provided in the test plans for each of the two categories. However, to address EPA's comments, PCA will provide data from testing currently being performed by one of its members on monomer acid sodium salt. Monomer acid sodium salt readily dissociates into monomer acid under aqueous conditions, so that the test data should be adequate for information regarding the properties of monomer acid. Data on monomer acid sodium salt should also be representative of octadecanoic acid due to their similarity in composition. (Octadecanoic acid is simply the hydrogenated form of monomer.) Moreover, since EPA's HPV Guidelines for grouping chemicals into a category endorse the use of the "family approach" of examining related acids and acid salts, the proposed testing of the monomer acid sodium salt as a surrogate for monomer acid is appropriate and should address EPA's concerns.

EPA also noted that it would be helpful to confirm that the branched and cyclic constituents present in the various category members arise in the processing of tall oil fatty acids to other products. Based on our knowledge of the chemistry of the formation of monomer acid, the cyclic structures in monomer are predominantly 1,2-disubstituted six-membered rings that arise from the cyclization of the linoleic and linolenic acids present in TOFA. The formation of cyclic acids in monomer acid is analogous to the well-documented formation of these same structures in heated vegetable fats such as soybean, linseed, and sunflower except that the reaction is acid-catalyzed rather than occurring through a radical mechanism as in the case of heated oils.

Amendment to Test Plan:

Robust summaries of data on both TOFA and monomer acid sodium salt will be provided for this category. Rather than amend every section of the Test Plan, the revised Table 1 below incorporates the testing to be performed on monomer acid sodium salt, as well as provides a complete picture of the testing to be performed under this Test Plan.

Table 1
Matrix of Available Adequate Data and Proposed Testing On Tall Oil Fatty Acids and Tall Oil Fatty Acid Salts*

Chemical and CAS #	Required SID Endpoints										
	Partition Coef.	Water Sol.	Biodeg.	Acute Fish	Acute Daph.	Acute Algae	Acute oral	Repeat Dose	In vitro genetox (bact.)	In vitro genetox non-bact	Repro/ develop
61790-12-3, Fatty acids, tall-oil	Adeq.	Test	Adeq.	Test	Test	Test	Adeq.	Adeq.	Adeq.	Adeq.	Adeq./ Adeq.
65997-03-7, Fatty acids, tall-oil, low boiling	Adeq.	Test	Adeq.	C	C	C	C	C	C	C	C
68955-98-6, Fatty acids, C16-C18 and C18 unsat., branched & linear#	Test	Test	Test	Test	Test	Test	Test	Test	Test	Test	Test
68201-37-6, Octadecanoic acid, branched and linear	Test	Test	Test	C	C	C	C	C	C	C	C
61790-44-1, Fatty acids, tall oil, potassium salts	Test	Test	Adeq.	C	C	C	C	C	C	C	C
61790-45-2, Fatty acids, tall oil, sodium salts	Test	Test	Test	C	C	C	C	C	C	C	C

Adeq. Indicates adequate existing data
Test Indicates proposed testing
C Indicates category read-down from existing or proposed test data on either tall oil fatty acid or fatty acids, C16-C18 and C18 unsaturated, branched & linear (i.e., monomer acid)
* No testing will be conducted for melting point, boiling point, vapor pressure, hydrolysis, photodegradation, and transport and distribution between environmental compartments as explained in the test plan.
\# The sodium salt of fatty acids, C16-C18 and C18 unsaturated, branched & linear (i.e., monomer acid sodium salt) will be tested as a surrogate for monomer acid.

Physicochemical Data - Vapor Pressure

PCA's Test Plan points out that the vapor pressure of all members of the TOFA category are negligible, so that experimental measurement is not meaningful. EPA agreed with PCA that the vapor pressure for salts in this category would be negligible, but did not present its views on the non-salts. Nonetheless, as an alternative to measuring the vapor pressure of the sponsored chemicals, EPA recommended that PCA measure the vapor pressure of "the most volatile fatty acid components, or at least for the major constituents of these [sponsored] chemicals."

PCA disagrees with this recommendation. Even the "most volatile fatty acid component" of the sponsored chemicals has a negligible vapor pressure that is essentially zero at ambient temperature and pressure. In addition, measuring the vapor pressure of the components of the substances will not provide relevant information on the substances that PCA has agreed to sponsor in the HPV program. Rather, it will provide information on chemicals that are outside of PCA's commitment (i.e., substances with different CAS numbers). Notably, however, another consortium has agreed to sponsor chemicals that comprise some of the major constituents (see Soap and Detergent Association (SDA) consortia commitments). Thus, EPA will obtain extensive physicochemical data on some of the components of the complex mixtures in this category, albeit from a different source.

Environmental Fate & Pathways - Photodegradation

EPA also suggests that PCA should measure photodegradation of the constituents of the sponsored chemicals. As stated above, PCA's sponsorship commitment runs to the specific Class 2 substances in the TOFA category and not their individual constituents which have been sponsored through SDA. Testing of constituents would not represent the properties of the sponsored chemicals. Consequently, determination of photodegradation of the constituents will not be undertaken.

Environmental Fate - Transport & Distribution

EPA noted that PCA did not discuss transport/distribution (also known as fugacity) data in the April 2001 Test Plan. Fugacity modeling is inappropriate for complex Class 2 substances such as TOFA and related substances, because the required inputs are either not available or are not feasible to determine. Consequently, fugacity modeling will not be undertaken. The Test Plan is hereby amended as follows to address this issue.

Amendment to Test Plan:

The transport and distribution between environmental compartments is intended to determine the ability of a chemical to move or partition in the environment. The determination of this property requires the use of various models (e.g., level III model from the Canadian Environment Modeling Centre at Trent University). For Class 2 substances such as TOFA and related substances, the required inputs to the model are either not available or not feasible to determine, including molecular mass, reaction half-life estimates for air, water, soil, sediment, aerosols, suspended sediment, and aquatic biota. In addition, the partition coefficient is also required, but the multiple K_{ow} values typically derived for these substances are a consequence of sample fractionation and reflect various components in the mixture and are not representative of the mixture itself. For example, at pH 2 and 7.5 there are seven and six K_{ow} values, respectively, for TOFA. Consequently, due to the inability to provide usable inputs to the required model for the specific substances in the TOFA category, determination of transportation and distribution between environmental compartments will not be undertaken for TOFA and related substances.

Ecotoxicity Tests

EPA agreed with the proposed acute toxicity testing of fish and algae, but suggested PCA conduct a 21-day chronic daphnid reproduction test using a flow-through method with measured concentrations. In contrast, PCRM recommended that PCA omit its proposed aquatic toxicity testing because "the properties of the tall oil fatty acids make aquatic toxicity tests meaningless."

After consideration of these comments, PCA does not intend to amend its Test Plan with regard to the proposed ecotoxicity testing. The methodology for preparing the water for PCA's ecotoxicity testing is identical to that used to determine solubility. This procedure was adopted in order to ensure that testing was conducted at the limit of actual water solubility. Given the extremely low solubility of the material, EPA's recommendation for a 21-day test using a flow-through method would be impracticable. Based on the amount of water that would be required and the difficulty in performing the necessary serial analytical measurements, a flow-through test for TOFA and related substances is simply not feasible. In addition, where there is a risk of emulsions forming inherently (as there might be with TOFA), flow through testing in not possible and is not recommended pursuant to the OECD (2000) Guidance Document 23 (Aquatic Toxicity Testing of Difficult Substances and Mixtures), which EPA specifically recommends PCA should follow. Thus, chronic aquatic toxicity testing in daphnia is not appropriate for this substance.